Math 540 - Assignment 2

Lewis Blake

March 19, 2019

Contents

1 Introduction

The main task in this assignment is to use parallel (Fortran or C or C++) programming with MPI to evaluate highly-oscillatory integrals by letting each allocated processing core in a communicator to compute only mildly-oscillatory integrals, for all chosen wavenumbers. Let K be a fixed wavenumber. Let $f(K, \cdot) : [a, b] \to \mathbb{R}$ be a highly oscillatory function. (Think of, or plot $f(K, x) = \cos(Kx), x \in [0, \pi]$ for $K = 1000$.)

Let

$$H(K) = \int_a^b f(K, x)\, dx.$$

Identify K naturally parallel tasks $A(K, i)$ (through constants a_i, b_i) for $i = 1, ..., K$ so that

$$H(K) = \int_a^b f(K, x) dx = \sum_{i=1}^{K} \int_{a_i}^{b_i} f(K, x)\, dx =: \sum_{i=1}^{K} A(K, i)$$

and for each $i = 1, ..., K$ the partial integral $A(K, i)$ is an integral of $f(K, \cdot)$ on $[a_i, b_i]$ of width $(b_i - a_i)/K$. Write down a_i, b_i for $i = 1, ..., K$.

Partition each interval $[a_i, b_i]$, $i = 1, ..., K$, using a fixed number $n + 1$ of (quadrature) points:

$$a_i = x_{i,0} < x_{i,1} < x_{i,2} < \cdots < x_{i,n} = b_i.$$

Let

$$\xi_{i,j} = \frac{x_{i,j-1} + x_{i,j}}{2}, \quad h_{i,j} = x_{i,j} - x_{i,j-1}, \quad i = 1, \cdots, K, \quad j = 1, \cdots n.$$

For each fixed K and $i = 1, ..., K$, consider three distinct approximations to $A(K, i)$ denoted by $A_{M,n}(K, i), A_{T,n}(K, i)$, and $A_{S,n}(K, i)$ where the mid-point (M), trapezoid (T), and Simpson's (S) rule approximations with the $n + 1$ quadrature points are defined by

$$A_{M,n}(K, i) = \sum_{j=1}^{n} f(K, \xi_{i,j})\, h_{i,j}, \quad A_{T,n}(K, i) = \sum_{j=1}^{n} \frac{1}{2} \left[f(K, x_{i,j-1}) + f(K, x_{i,j}) \right] h_{i,j}$$

$$A_{S,n}(K, i) = \frac{2}{3} A_{M,n}(K, i) + \frac{1}{3} A_{T,n}(K, i).$$

2 Problem 1

Write a procedure with dummy input variables being

- an external integrand function, say, fn (which is assumed to be a function of two variables; wavenumber is the first variable).
- a wavenumber, say, w_n
- a vector of quadrature points, say, pts (with starting index 0
- and the total number of quadrature pts, say $q_n + 1$

and the output variables being M, T, S that are computed using the formulas:

$S = \frac{2}{3}M + \frac{1}{3}T$

$M = \sum_{j=1}^{q_n} fn\,(w_n, mpts)\, \mathrm{len}(j), \quad T = \sum_{j=1}^{q_n} \frac{1}{2} \left[fn\,(w_n, pts(j-1)) + fn\,(w_n, pts(j)) \right] \mathrm{len}(j)$

where $len(j) = pts(j) - pts(j-1), \quad mpts(j) = (pts(j) + pts(j-1))/2 \quad j = 1, \cdots, q_n$

2.1 Problem 1 Solution

Please see `evaluateA()` in `assign2.cpp`.

3 Problem 2

Write a procedure with dummy input variables being a vector, say, *points*, its size *ptsize*, a wavenumber, say, k_w and the output being a vector fun_val_points, defined by

$$fun\_val\_points = \cos\left(100 * points - k_w * \sin(points)\right).$$

3.1 Problem 2 Solution

Please see `evaluateFunction()` in `assign2.cpp`.

4 Problem 3

Using the procedures in Q.1 and Q.2, write a main program with MPI to compute for each of the 9901 integer wavenumbers in $K \in [100, 10000]$, (with a total number of processing cores P) defined in a load balanced way, three distinct approximation values for

$$H(K) = \int_0^\pi f(K,x)dx, \quad f(K,x) = \cos(100x - K\sin(x)),$$

with 101 *equally spaced* quadrature points on each $[a_i, b_i]$, for $i = 1, ..., K$, denoted by $H_{M,100}(K), H_{T,100}(K), H_{S,100}(K)$ where (using the notation introduced earlier)

$$H_{M,100}(K) = \sum_{i=1}^{K} A_{M,100}(K,i), \quad H_{T,100}(K) = \sum_{i=1}^{K} A_{T,100}(K,i), \quad H_{S,100}(K) = \sum_{i=1}^{K} A_{S,100}(K,i).$$

Your parallel main program with MPI (parallelizing the naturally tasks for each K) should:

- Print out, in a four column table, ten wavenumbers $K = 1000, 2000, \cdots, 10000$ and associated approximations $H_{M,100}(K), H_{T,100}(K)$ and $H_{S,100}(K)$, with appropriate headings including the total number P of cores used in computation. (Submit the tabulated values obtained using $P = 8$ and $P = 16$ cores.)

- You may use the following high-order approximate values to make sure that your computed values match at least a few digits of these given values:
$H(100) \approx 3.027448328771664E-01, \quad H(1100) \approx -3.675617781869349E-02$
Use the format in these numbers and the table below as a sample for your print out format and headings.

- Save the approximate values of $H(K)$ for $K = 100, 101, \cdots, 10,000$ in a file to facilitate plotting the functions, $H_{M,100}, H_{T,100}$ and $H_{S,100}$ on $[100, 10000]$

4.1 Problem 3 Solution

Please see Table 1 and Table 2.

Table 1: Approximations to oscillatory integrals computed using $P = 8$ cores.

K	Midpoint_H(K)	Trapezoid_H(K)	Simpson's_H(K)
1000	3.6681659962834547e-02	3.6681659962834200e-02	3.6681659962834422e-02
2000	-4.8656584015455306e-02	-4.8656584015454779e-02	-4.8656584015455112e-02
3000	-3.6152554160266387e-02	-3.6152554160266984e-02	-3.6152554160266581e-02
4000	-1.3726571727345186e-02	-1.3726571727346117e-02	-1.3726571727345496e-02
5000	1.2816974994247750e-02	1.2816974994247957e-02	1.2816974994247820e-02
6000	2.9882648822820736e-02	2.9882648822823207e-02	2.9882648822821559e-02
7000	2.6841063851925619e-02	2.6841063851924606e-02	2.6841063851925296e-02
8000	6.2827840283860249e-03	6.2827840283868333e-03	6.2827840283862894e-03
9000	-1.6573327811025943e-02	-1.6573327811026738e-02	-1.6573327811026210e-02
10000	-2.5058965045117555e-02	-2.5058965045118030e-02	-2.5058965045117725e-02

Table 2: Approximations to oscillatory integrals computed using $P = 16$ cores.

K	Midpoint_H(K)	Trapezoid_H(K)	Simpson's_H(K)
1000	3.6681659962834547e-02	3.6681659962834193e-02	3.6681659962834429e-02
2000	-4.8656584015455320e-02	-4.8656584015454786e-02	-4.8656584015455112e-02
3000	-3.6152554160266380e-02	-3.6152554160266998e-02	-3.6152554160266588e-02
4000	-1.3726571727345189e-02	-1.3726571727346114e-02	-1.3726571727345500e-02
5000	1.2816974994247750e-02	1.2816974994247953e-02	1.2816974994247816e-02
6000	2.9882648822820740e-02	2.9882648822823203e-02	2.9882648822821562e-02
7000	2.6841063851925615e-02	2.6841063851924640e-02	2.6841063851925275e-02
8000	6.2827840283860240e-03	6.2827840283868402e-03	6.2827840283862964e-03
9000	-1.6573327811025936e-02	-1.6573327811026734e-02	-1.6573327811026210e-02
10000	-2.5058965045117558e-02	-2.5058965045118033e-02	-2.5058965045117731e-02

5 Problem 4

Plot your approximate, $H_{M,100}$, $H_{T,100}$, $H_{S,100}$ computed using 16 cores and submit three plots.

5.1 Problem 4 Solution

Please see Figure 1 for each of these plots.

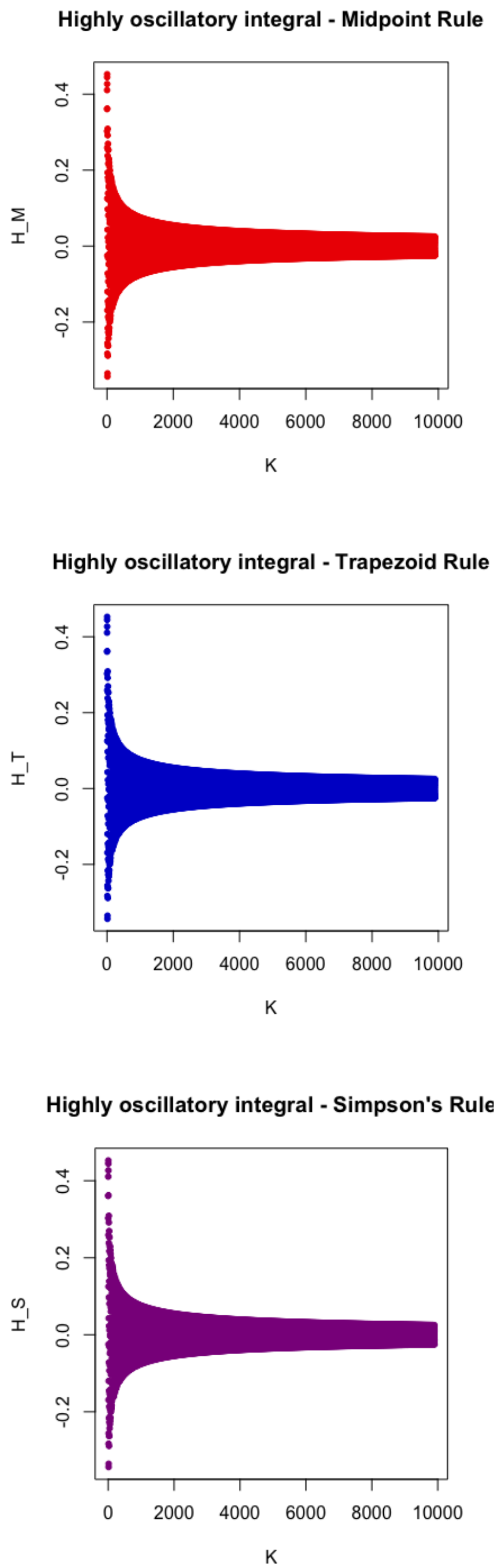

Figure 1: Plot of the highly oscillatory integrals approximations as a function of their wave number (K).